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Topological susceptibility in staggered fermion chiral perturbation theory

Brian Billeter, Carleton DeTar, and James Osborn
Physics Department, University of Utah, Salt Lake City, Utah 84112, USA
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The topological susceptibility of the vacuum in quantum chromodynamics has been simulated numerically using the Asqtad improved staggered fermion formalism. At nonzero lattice spacing, the residual fermion doublers (fermion tastes) in the staggered fermion formalism give contributions to the susceptibility that deviate from conventional continuum chiral perturbation theory. In this brief report, we estimate the taste-breaking artifact and compare it with results of recent simulations, finding that it accounts for roughly half of the scaling violation.

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I. INTRODUCTION

The staggered fermion formalism reduces the number of fermion doublers to four species ("tastes") per quark flavor. At zero quark mass in the continuum limit, the taste-symmetry group becomes $SU(4)_L \times SU(4)_R \times U(1)_V$, but at nonzero lattice spacing this symmetry is broken by lattice-artifact, taste-changing interactions. Taste-breaking effects modify predictions of chiral perturbation theory, complicating efforts to extrapolate lattice results simultaneously to zero quark mass and zero lattice spacing. However, a recently developed modification to chiral perturbation theory, called "staggered chiral perturbation theory (SχPT)," permits a quantitative treatment of taste-breaking effects [1,2]. Combining these modifications with an improved staggered fermion formulation that substantially reduces the strength of taste-breaking has proven highly effective in carrying out high-precision extrapolations of results from lattice simulations [3].

In this brief report, we use staggered chiral perturbation theory to predict the topological susceptibility. The derivation is given in Sec. II, and in Sec. III the resulting formula is compared with results of recent lattice simulations with improved staggered fermions.

II. TOPOLOGICAL SUSCEPTIBILITY WITH TASTE-SYMMETRY BREAKING

We consider the low energy effective chiral Lagrangian for N flavors of staggered fermions, each with four tastes. The Lagrangian is written in terms of the $(4N)^2$ pseudoscalar meson fields ϕ_{ia}, encapsulated in a unitary $4N \times 4N$ matrix:

$$U = \exp(iT_{ia}\phi_{ia}/f). \tag{1}$$

We use $f \approx 130$ MeV. We label the generators of the Lie algebra of U(4N) with a flavor index i and taste index a and write them as

$$T_{ia} = \Lambda_i t_a, \tag{2}$$

where the t_a, the 16 taste matrices (Dirac gamma matrices plus the identity), are enumerated as

$$\xi_5, \xi_\mu, i\xi_{\mu 5} = i\xi_\mu \xi_5, i\xi_{\mu\nu} = i\xi_\mu \xi_\nu, \xi_I = I, \tag{3}$$

and the Λ_i are the N^2 generators of U(N). The t_a are orthonormal:

$$\mathrm{Tr}(t_a t_b) = 4\delta_{ab}, \tag{4}$$

but we normalize the Λ_i so that

$$\mathrm{Tr}(\Lambda_i \Lambda_j) = \delta_{ij}. \tag{5}$$

Moreover, for convenience we choose a quark flavor basis in which the diagonal generators are enumerated first and are explicitly

$$(\Lambda_i)_{jk} = \delta_{ij}\delta_{ik} \quad \text{for } i = 1, \ldots, N. \tag{6}$$

Also, for convenience, we define the flavor-singlet generator and fields

$$\Lambda_0 = I, \tag{7}$$

$$\phi_{0a} = \sum_{i=1}^{N} \phi_{ia}/\sqrt{N}. \tag{8}$$

The Euclidean Lee-Sharpe SχPT Lagrangian [1], extended by Aubin and Bernard to N flavors [2] and including an explicit mass term for the anomalous flavor-singlet field, is

$$\begin{aligned}\mathcal{L} &= \frac{f^2}{8}\mathrm{Tr}(\partial_\mu U^\dagger \partial_\mu U) - \frac{\mu f^2}{4}\mathrm{Tr}[\mathcal{M}(U^\dagger + U)] \\ &\quad + \frac{m_0^2}{2}\phi_{0I}^2 + a^2\mathcal{V}(U),\end{aligned} \tag{9}$$

where a is the lattice spacing, the trace is over all $4N$ taste and flavor indices, $\mathcal{M}$ is the taste-degenerate quark mass matrix,

$$\mathcal{M}_{ia,jb} = M_{ij}\delta_{ab} = \delta_{ij}\delta_{ab}m_i, \tag{10}$$

and the taste-breaking potential,

$$-\mathcal{V}(U) = \sum C_i \mathcal{O}_i, \tag{11}$$

is a linear combination of the operators,

$$\mathcal{O}_1 = \mathrm{Tr}(T_{0,5}UT_{0,5}U^\dagger), \tag{12}$$

$$\mathcal{O}_{2V} = \tfrac{1}{4}[\mathrm{Tr}(T_{0,\mu}U)\mathrm{Tr}(T_{0,\mu}U) + \mathrm{H.c.}], \tag{13}$$

$$\mathcal{O}_{2A} = \tfrac{1}{4}[\mathrm{Tr}(T_{0,\mu 5}U)\mathrm{Tr}(T_{0,5\mu}U) + \mathrm{H.c.}], \tag{14}$$

$$\mathcal{O}_3 = \tfrac{1}{2}[\mathrm{Tr}(T_{0,\mu}UT_{0,\mu}U) + \mathrm{H.c.}], \tag{15}$$

$$\mathcal{O}_4 = \tfrac{1}{2}[\mathrm{Tr}(T_{0,\mu 5}UT_{0,5\mu}U) + \mathrm{H.c.}], \tag{16}$$

$$\mathcal{O}_{5V} = \tfrac{1}{2}[\mathrm{Tr}(T_{0,\mu}U)\mathrm{Tr}(T_{0,\mu}U^\dagger)], \tag{17}$$

$$\mathcal{O}_{5A} = \tfrac{1}{2}[\mathrm{Tr}(T_{0,\mu 5}U)\mathrm{Tr}(T_{0,5\mu}U^\dagger)], \tag{18}$$

$$\mathcal{O}_6 = \sum_{\mu<\nu}\mathrm{Tr}(T_{0,\mu\nu}UT_{0,\nu\mu}U^\dagger). \tag{19}$$

The partition function is, as usual,

$$Z = \int [dU]\exp\Big(-\int \mathcal{L}\, dV\Big). \tag{20}$$

The chiral condensate is defined by

$$\Sigma_i = \lim_{m_i\to 0}\frac{1}{4}\frac{\partial \log Z}{\partial m_i}, \tag{21}$$

and is, as usual,

$$\Sigma_i = \Sigma = \mu f^2/2. \tag{22}$$

The bare meson masses are obtained by expanding the Lagrangian to quadratic order in the meson fields:

$$\mathcal{L} = \frac{1}{2}\sum_{ia}(\partial_\mu\phi_{ia})^2 + \frac{1}{2}\sum_{iajb}A_{ia,jb}\phi_{ia}\phi_{jb}, \tag{23}$$

where the flavor and taste-mixing matrix is

$$A_{ia,jb} = A^{(0)}_{ij}\delta_{ab} + A^{(1)}_{ij}\delta_{Ia}\delta_{Ib} + a^2 B_{ab}\delta_{ij}. \tag{24}$$

The continuum taste-singlet flavor-mixing matrix is block diagonal with an invariant subspace $i = 1, 2, \ldots, N$. This is the only subspace that contributes to the tree-level topological susceptibility. For i, j in this set we have

$$A^{(0)}_{ij} = 2\mu\,\mathrm{Tr}(M\Lambda_i\Lambda_j) = 2\mu\,\delta_{ij}m_i, \tag{25}$$

$$A^{(1)}_{ij} = m_0^2/N. \tag{26}$$

The flavor-singlet taste-mixing matrix B_{ab} is defined by the small field expansion,

$$\mathcal{V}(U) \approx \frac{1}{2}\sum_{i,a,b}B_{ab}\phi_{ia}\phi_{ib}. \tag{27}$$

Without the anomalous mass term m_0^2 and without taste breaking, the bare flavor-neutral meson masses are given by the diagonal values in $A^{(0)}$:

$$m^2_{ia} = 2\mu m_i \quad \text{for } i = 1, 2, \ldots, N. \tag{28}$$

To lowest order in the taste-breaking potential, the pseudoscalar mass splittings were calculated by Lee and Sharpe [1]. With the Aubin and Bernard generalization [2], they are

$$\Delta m^2_{ia} = a^2\Delta_a, \tag{29}$$

where $\Delta_a = B_{aa}$ and

$$\Delta_5 = 0, \tag{30}$$

$$\Delta_\mu = \frac{16}{f^2}(C_1 + C_3 + 3C_4 + 3C_6), \tag{31}$$

$$\Delta_{\mu 5} = \frac{16}{f^2}(C_1 + 3C_3 + C_4 + 3C_6), \tag{32}$$

$$\Delta_{\mu\nu} = \frac{16}{f^2}(2C_3 + 2C_4 + 4C_6), \tag{33}$$

$$\Delta_I = \frac{16}{f^2}(4C_3 + 4C_4). \tag{34}$$

To formulate the topological susceptibility in the presence of taste breaking, we recall the derivation, starting from the quark and gluon Lagrangian $\mathcal{L}_{\mathrm{QCD}}$. The partition function receives contributions from topological charge sectors ν as follows [4]:

$$Z = \sum_\nu Z_\nu, \tag{35}$$

where the microcanonical partition function is

$$Z_\nu = \int dq\, d\bar{q}\, dA\, d\theta \exp(-i\theta\nu)\exp\Big(\int[\mathcal{L}_{\mathrm{QCD}} + i\theta F\tilde{F}/64\pi^2]\,dV\Big). \tag{36}$$

The theta term in the Lagrangian can be removed by a flavor (and taste) singlet $U_A(1)$ chiral rotation, leaving a Lagrangian $\mathcal{L}_{\mathrm{QCD}}(\theta)$ with rotated quark fields. The lattice staggered fermion action breaks this symmetry through the quark mass term and through taste-symmetry breaking at nonzero lattice spacing a. To order a^2 in SχPT, the symmetry breaking is described by the $U_A(1)$ noninvariant taste-breaking term $a^2\mathcal{V}(U)$. The $U_A(1)$ rotation on the quark fields is modeled in the effective theory by the corresponding rotation on the meson matrix U:

$$\mathcal{L}(\theta) = \frac{f^2}{8}\mathrm{Tr}(\partial_\mu U^\dagger\partial_\mu U) - \frac{\mu f^2}{4}\mathrm{Tr}[\mathcal{M}(e^{-i\theta/4N}U^\dagger + e^{i\theta/4N}U)] + \frac{m_0^2}{2}\phi_{0I}^2 + a^2\mathcal{V}(e^{i\theta/4N}U). \tag{37}$$

A field redefinition $\phi_{iI} \to \phi_{iI} - f\theta/4N$ for $i = 1, \ldots, N$, implying $\phi_{0I} \to \phi_{0I} - f\theta/4\sqrt{N}$, gives an alternate expression,

$$\mathcal{L}(\theta) = \frac{f^2}{8}\mathrm{Tr}(\partial_\mu U^\dagger\partial_\mu U) - \frac{\mu f^2}{4}\mathrm{Tr}[\mathcal{M}(U^\dagger + U)] + \frac{m_0^2}{2}\times(\phi_{0I} - f\theta/4\sqrt{N})^2 + a^2\mathcal{V}(U). \tag{38}$$

We work in the mean-field ϵ regime in which the fields are space and time independent and take the limit $m\Sigma V \to \infty$, and $m_0^2 V \to \infty$, i.e., asymptotically large mean square topological charge $\langle \nu^2 \rangle$. In this limit, we may use a saddle-point approximation to compute the microcanonical partition function. The saddle-point occurs close to the identity in U and origin in θ, where we replace the Haar measure dU with the $(4N)^2$ dimensional Cartesian measure $d\phi$ and expand the integrand to quadratic order in the meson field ϕ and θ:

$$Z_\nu \propto \int d\phi \, d\theta \exp(-i\theta\nu) \times \exp\left\{-\frac{V}{2}[F(\phi) + m_0^2(\phi_{0I} - f\theta/4\sqrt{N})^2]\right\}, \tag{39}$$

where $F(\phi)$ is the quadratic form,

$$F(\phi_{ia}) = \sum_{ia,jb}[A_{ij}^{(0)}\delta_{ab} + a^2 B_{ab}\delta_{ij}]\phi_{ia}\phi_{jb}. \tag{40}$$

The only meson fields contributing to the susceptibility are the diagonal taste-singlet mesons ϕ_{iI} for $i = 1, 2, \ldots, N$. The corresponding subspace is invariant under the quadratic form. Thus, the remaining fields can be integrated out immediately. The integration over theta gives

$$Z_\nu \propto \int \prod_{i=1}^{N} d\phi_{iI} \exp(-i4\sqrt{N}\phi_{0I}\nu/f) \times \exp\left[-\frac{V}{2}F(\phi_{iI}) - 16N\nu^2/(2Vf^2m_0^2)\right], \tag{41}$$

and finally the integration over taste-singlet meson fields gives

$$Z_\nu \propto \exp\left[-16\nu^2 \Big/ \left(2Vf^2 \sum_{i=1}^{N} 1/m_{iI}^2\right) - 16N\nu^2/(2Vf^2m_0^2)\right], \tag{42}$$

where the bare taste-shifted flavor-neutral masses are

$$m_{iI}^2 = 2\mu m_i + a^2\Delta_I. \tag{43}$$

The resulting topological susceptibility is

$$\chi = \langle \nu^2 \rangle / V = \frac{f^2/16}{\sum_{i=1}^{N} 1/m_{iI}^2 + N/m_0^2}. \tag{44}$$

When the N flavors can be grouped into p degenerate flavor multiplets with degeneracy n_k so that $\sum_{k=1}^{p} n_k = N$, the susceptibility is

$$\chi = \langle \nu^2 \rangle / V = \frac{f^2/16}{\sum_{k=1}^{p} n_k(1/m_{kI}^2 + 1/m_0^2)}. \tag{45}$$

Counting the taste symmetry as well, the continuum limit degeneracy of quark species is then $4n_k$ for each distinct flavor. In numerical simulations of staggered fermions, it is necessary to take fractional powers of the quark determinant to simulate a theory with the physical count of 2 + 1 flavors, i.e., only two species of light u and d quarks of the same mass and a single s quark. The SχPT treats only the case in which quark multiplets come in multiples of four. Absent a rigorous treatment of fractional powers in SχPT, we adopt the replica trick: Assume that an analytic continuation in the flavor number n_k reproduces the effect of taking a fractional power of the determinant. That is, we replace $4n_{ud}$ by 2 and $4n_s$ by 1 in the expression above. The susceptibility for 2 + 1 flavors is then

$$\chi = \frac{f^2 m_{\pi,I}^2/8}{1 + m_{\pi,I}^2/2m_{ss,I}^2 + 3m_{\pi,I}^2/2m_0^2}. \tag{46}$$

Of course, this result is valid only in leading order chiral perturbation theory, but at large quark mass it interpolates smoothly [5] to the quenched result predicted for pure gauge theory [6].

$$\chi_q = f^2 m_0^2/12. \tag{47}$$

At small m_{ud}, the susceptibility is dominated by the pion mass. Without taste breaking we recover the conventional formula,

$$\chi = f^2 m_\pi^2/8. \tag{48}$$

We see that the effect of taste breaking at leading order is simply to replace the masses of the Goldstone mesons in the conventional expression with the masses of the corresponding taste-singlet non-Goldstone states. The squared masses of these states vary linearly with quark mass and have a nonzero intercept. Therefore, at nonzero lattice spacing, the topological susceptibility does not vanish at zero quark mass. However, in the continuum limit, the expected zero is recovered.

III. COMPARISON WITH SIMULATION RESULTS

The topological susceptibility has been determined recently for gauge configurations generated with an improved staggered fermion action [7]. It was found that at nonzero lattice spacing the lattice susceptibility is higher than that predicted by chiral perturbation theory, but (at least within the available statistical errors and an extrapolation based on limited data) it is consistent with the continuum prediction. Two principal causes for disagreement at nonzero lattice spacing were proposed: (i) Dislocations in the gluon field could imitate small instantons and participate in screening of the topological charge. These and small instantons are erased in the smoothing (cooling) process, possibly leaving behind larger, unscreened instantons. The latter would then increase the smoothed susceptibility. (ii) The would-be zero modes are not at zero because of taste-symmetry break-

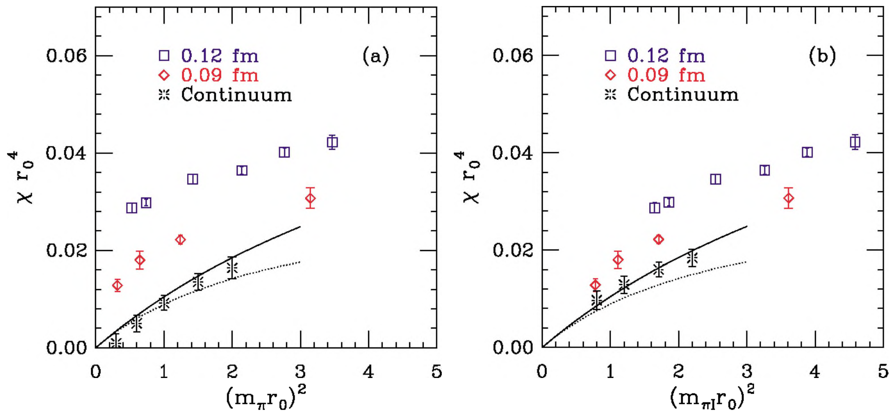

FIG. 1 (color online). Topological susceptibility vs pion mass squared in units of r_0 with improved (Asqtad) staggered quarks. Data is from Ref. [7], reanalyzed with a new variance reduction method and new 0.09 fm data point [8]: (a) plotted as a function of the Goldstone pion mass squared; (b) replotted as a function of the taste-singlet pion mass squared. The bursts show the continuum extrapolation at fixed abscissa in each case. The solid line shows the prediction of leading order continuum chiral perturbation theory [Eq. (46)] without the $U(1)$ mass term m_0^2. The dashed line includes m_0^2, determined through Eq. (47) from the simulated quenched susceptibility [8].

ing, so are not fully effective in suppressing the topological charge at small quark mass. The latter effect is taken into account in Eq. (46).

In light of our result [Eq ((46)] we replot reanalyzed data of Ref. [7] as a function of the taste-singlet pion mass $m_{\pi,I}^2 r_0^2$ in Fig. 1(b). For comparison, the same data is plotted as a function of the Goldstone pion mass $m_\pi^2 r_0^2$ in Fig. 1(a). The reanalysis is described in detail elsewhere [8]. In this work we are concerned with the taste-breaking artifact.

We see that correcting for staggered fermion artifacts removes roughly half the scaling violation in this range of pion masses. The rest can be attributed to the definition of the topological charge density operator, including smoothing [7]. It is plausible that those corrections decrease as $\mathcal{O}(a^2)$. We assume this form in carrying out the rough continuum extrapolation. The extrapolation to the continuum starts by fitting the measured points for each lattice spacing to the curve $1/\chi = c/m_{\pi,I}^2 + b$ and then performing an extrapolation linearly in a^2 of the thus smoothed values of χ. In the left panel, the extrapolation was done at constant Goldstone pion mass m_π^2; in the right panel, at fixed $m_{\pi,I}^2$. Because staggered fermion artifacts contribute to scaling violations at fixed Goldstone pion mass, and those artifacts decrease as $\mathcal{O}(\alpha_s^2 a^2)$, rather than $\mathcal{O}(a^2)$, the extrapolation in Fig. 1(a) is somewhat less plausible than the extrapolation in Fig. 1(b).

To make further progress, we need simulations at a smaller lattice spacing.

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